2025 Volume: 01 Issue: 07 www.ijrpa.com ISSN 2456-9995 Review Article

International Journal Research Publication Analysis

Page: 01-12

MARMESIN: A MULTIFUNCTIONAL FURANOCOUMARIN BRIDGING NATURAL PRODUCT CHEMISTRY AND PHARMACOLOGICAL INNOVATION

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Received: 23 November 2025
Article Revised: 13 December 2025
Published on: 03 January 2026

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DOI: https://doi-doi.org/101555/ijrpa.8850

ABSTRACT

Marmesin, a naturally derived furanocoumarin, has attracted considerable scientific interest due to its extensive pharmacological potential. Isolated from various medicinal plants including *Aegle marmelos*, *Broussonetia kazinoki*, and *Feronia limonia*, this bioactive molecule demonstrates a wide range of therapeutic effects encompassing anticancer, anti-inflammatory, antidiabetic, hepatoprotective, antimicrobial, and photobiological activities. Mechanistic studies indicate that marmesin exerts its pharmacological actions by modulating several key molecular targets such as PI3K/Akt and VEGF-A pathways, and by inhibiting enzymes like COX-2, 5-LOX, and aldose reductase. It also enhances insulin secretion by regulating β-cell signaling and exhibits inhibitory activity against human heparan sulfatase-2 (HSULF-2), a known cancer-related enzyme. The broad therapeutic profile of marmesin highlights its potential as a natural lead molecule for drug discovery. This review consolidates existing literature on its structural characteristics, sources, biological activities, and mechanisms of action, emphasizing its emerging importance in modern pharmacological research.

BACKGROUND

Furanocoumarins are a distinctive group of naturally occurring secondary metabolites characterized by the fusion of a furan ring with a coumarin nucleus. These compounds,

widely distributed in the **Apiaceae** and **Rutaceae** plant families, are known for their photoreactive and bioactive properties. Traditionally, furanocoumarins have been associated with phototherapy and plant defense mechanisms; however, their diverse pharmacological potential has gained significant attention in recent years.

Among these compounds, **marmesin**, a dihydrofurocoumarin derivative, has emerged as a molecule of considerable therapeutic interest. Originally recognized as a biosynthetic precursor of linear furanocoumarins such as psoralen, marmesin has now been established as a pharmacologically active compound in its own right. It exhibits multiple biological effects including anticancer, antimalarial, anti-inflammatory, antioxidant, and hepatoprotective properties. These activities are attributed to its ability to modulate several cellular pathways and enzymatic systems involved in inflammation, oxidative stress, and cellular proliferation. Furthermore, studies have demonstrated that marmesin influences angiogenic processes by suppressing VEGF-A expression and inhibits critical enzymes like cyclooxygenase (COX) and lipoxygenase (LOX), which play a central role in inflammatory responses. Its ability to enhance insulin secretion and inhibit aldose reductase further underscores its potential in the management of met abolic disorders, particularly diabetes mellitus. In addition to its pharmacological versatility, marmesin's structural simplicity, natural abundance, and low toxicity make it a promising candidate for drug development.

Given its broad spectrum of biological effects, marmesin represents a valuable bridge between natural product chemistry and therapeutic innovation. The current review aims to provide a comprehensive overview of its chemical composition, biological activities, mechanisms of action, and pharmacological significance, establishing its role as a potent bioactive scaffold for the development of novel therapeutic agents.

KEYWORDS: Marmesin; Furanocoumarins; Anticancer; Anti-inflammatory; PI3K/Akt pathway; HSULF-2 inhibitor; Angiogenesis; Antidiabetic; Antimicrobial; Hepatoprotective activity; Natural product drug discovery.

INTRODUCTION

Furanocoumarins are a unique class of secondary metabolites characterized by the chemical fusion of a furan ring with a coumarin (benzopyrone) nucleus, forming either a partially or fully conjugated double bond system. This structural integration imparts distinct photoreactive and biological properties that differentiate them from other natural compounds.

These molecules are predominantly found in plants belonging to the Apiaceae (Umbelliferae) family and have been extensively studied for their diverse biological, ecological, and therapeutic roles.

According to **Shtratnikova (2023)**, research on furanocoumarins spans several decades, encompassing studies on their structural diversity, biosynthetic pathways, ecological functions in plants, and pharmaceutical potential. Their dual characteristics—acting as protective agents in plants and as bioactive compounds with therapeutic applications—continue to attract substantial interest across disciplines such as plant physiology, natural product chemistry, and pharmacology. Despite their known phototoxicity under light exposure, furanocoumarins remain valuable for drug discovery and biomedical research due to their wide range of pharmacological activities[1].

Impact of Furanocoumarins precursors on Herbivorous Insects

In an investigation by **Trumble and Millar (1996)**, the biological impact of two furanocoumarin precursors—demethylsuberosin and marmesin—was evaluated on the generalist herbivorous insect *Spodoptera exigua*. Their study revealed that neither compound significantly affected the insect's survival rate or developmental progression. However, a structurally related linear furanocoumarin, psoralen, exhibited marked effects by reducing growth rate and survival.

Interestingly, all three compounds demonstrated strong antifeedant properties, indicating their potential role in plant defense mechanisms. The larvae consistently avoided diets containing marmesin or psoralen, while demethylsuberosin also induced avoidance behavior, particularly in later larval stages. These findings suggest that although these precursor molecules are not overtly toxic, they function as effective feeding deterrents, helping plants protect themselves against herbivory[2].

Potential Antiplasmodial Properties of Marmesin and Celtis durandii

According to studies, Celtis durandii root extracts are effective against strains of Plasmodium falciparum, the parasite that causes malaria, that are both drug-sensitive and drug-resistant. From the extract, a more potent substance was separated and subsequently identified as marmesin. This substance suppressed the production of β-hematin, which is necessary for the parasite to survive, in addition to having potent antiplasmodial actions. According to these

results, marmesin and Celtis durandii may both be viable options for the creation of antimalarial medications **(Ezenyi et al., 2023)[3].**

Anticancer Effects of Bael Fruit Compounds (Marmesin and marmelosin) via HSULF-2 Inhibition

Human heparan sulfatase-2 (HSULF-2) is a cancer-related protein found in high amounts on the surface of many tumor cells, where it supports tumor growth and survival. **Hemakumar C et al. (2023)** investigated that extracts from bael fruit (*Aegle marmelos*), which are rich in phytochemicals such as marmesin and marmelosin, have demonstrated the ability to block HSULF-2 activity and promote the death of breast cancer cells. Computational analysis has further backed these findings by constructing a structural model of HSULF-2 and assessing its interaction with the plant-derived compounds. Docking studies showed that marmesin and marmelosin bind effectively to the active site of HSULF-2, and molecular dynamics simulations confirmed that these interactions remain stable over time. Together, these results provide strong evidence that bael fruit phytochemicals may act as natural inhibitors of HSULF-2, offering promising potential for cancer treatment[4].

Anticancer Potential of Marmesin in Esophageal Cancer

Marmesin, a coumarin compound derived from *Broussonetia kazinoki*, is known for various pharmacological effects, including potential anti-tumor activity. However, its impact on esophageal cancer (EC) remains unexplored. This study investigated the anti-cancer effects of marmesin on EC cell lines in vitro.

According to recent in vitro research by **Wang Q 2022 et al**, marmesin encourages apoptosis and inhibits the growth of esophageal cancer (EC) cells. Its anti-proliferative properties were validated by cell viability assays (CCK-8 and EdU), which were bolstered by a decrease in the expression of proliferation markers proliferating cell nuclear antigen (PCNA)and Ki67. TUNEL assays demonstrated apoptotic activity, which was linked to upregulated Bax and downregulated Bcl-2. The PI3K/Akt signaling pathway may be involved in the mechanism of action of marmesin, according to network pharmacology study. Reduced amounts of phosphorylated PI3K and Akt in treated cells served as confirmation of this. Furthermore, the effects of marmesin were reversed by overexpression of Akt, suggesting that the PI3K/Akt pathway is at least partially responsible for its anticancer action[5].

Natural Compounds Targeting the PI3K/Akt Pathway in Allergic Asthma: A Review

Recent studies have highlighted the therapeutic potential of natural compounds in regulating key inflammatory pathways involved in allergic asthma. In an ovalbumin (OVA)-induced asthma mouse model, a mixture of luteolin, arbutin, and marmesin significantly alleviated asthma symptoms by reducing serum IgE levels, pro-inflammatory cytokines (IL-4, IL-5, IL-13, TNF-α), and inflammatory cell infiltration in bronchoalveolar lavage fluid. Histopathological analysis confirmed mitigation of lung tissue damage, while apoptosis was reduced through downregulation of Bax and Caspase-3 and upregulation of Bcl-2. Importantly, the mixture suppressed the PI3K/Akt signaling pathway, as shown by decreased expression of PI3K, p-PI3K, and a reduced p-Akt/Akt ratio. These effects were comparable to those of the PI3K inhibitor LY294002 and the standard corticosteroid dexamethasone. The findings suggest that this active compound mixture exerts its anti-asthmatic effects primarily through inhibition of the PI3K/Akt pathway, offering a promising natural therapeutic strategy for the treatment of allergic asthma (**Liu C et al 2024)**[6].

Bioactive Constituents of *Angelica reflexa* Improve Insulin Secretion

This study aimed to identify bioactive compounds from *Angelica reflexa* that enhance glucose-stimulated insulin secretion (GSIS) in pancreatic β-cells. Three new compounds—koseonolin A (1), koseonolin B (2), and isohydroxylomatin (3)—along with 28 known compounds (4–31) were isolated from the roots of *A. reflexa* using chromatographic techniques. Structural elucidation of the new compounds was achieved through NMR, HRESIMS, and ECD analyses. The root extract (KH2E) and isolated compounds were evaluated for GSIS activity via GSIS assays, ADP/ATP ratio measurements, and Western blotting. KH2E significantly enhanced GSIS, with isohydroxylomatin (3), (−)-marmesin (17), and especially marmesinin (19) showing marked activity. Notably, marmesinin (19) exhibited a stronger effect on GSIS than gliclazide at the same concentration (13.21 ± 0.12 vs. 7.02 ± 0.32 at 10 μM). Marmesinin (19) upregulated key proteins involved in β-cell metabolism, including PPARγ, PDX-1, and IRS-2, and its effect was modulated by calcium and potassium channel regulators. These findings suggest that marmesinin (19) enhances insulin secretion via modulation of β-cell metabolic pathways and ion channels, highlighting its potential as a promising therapeutic candidate for type 2 diabetes **(Kim HS et al 2023)**[7]**.**

Marmesin is a novel angiogenesis inhibitor: Regulatory effect and molecular mechanism on endothelial cell fate and angiogenesisKim JH et al 2015

has investigated that, it has been shown to suppress vascular endothelial growth factor A (VEGF-A)-stimulated proliferation of human umbilical vein endothelial cells (HUVECs) by modulating cell cycle regulatory mechanisms. In a dose-dependent manner, marmesin significantly inhibited VEGF-A-induced cell proliferation without affecting overall cell viability, indicating that its anti-proliferative effects are not due to cytotoxicity or apoptosis. Flow cytometric analysis of DNA content revealed that VEGF-A stimulation increased the percentage of cells in the S and G2/M phases while reducing the G1 population, suggesting accelerated cell cycle progression. However, marmesin treatment reversed these effects, preventing the VEGF-A-induced G1 to S phase transition and causing cell cycle arrest in the G1 phase. Consistent with these observations, marmesin downregulated the expression of cyclin-dependent kinases (CDKs) and cyclin D, and led to hypophosphorylation of the retinoblastoma protein (pRb), thereby inhibiting cell cycle progression. These findings collectively suggest that marmesin exerts anti-angiogenic effects by arresting the endothelial cell cycle at the G1 phase through the suppression of key cell cycle regulators.

Marmesin inhibited endothelial cell migration**,** invasion, and tube formation in a dose-dependent manner. It significantly reduced the expression and activity of matrix metalloproteinase-2 (MMP-2), which plays a key role in extracellular matrix degradation and cell motility. In contrast, the levels of tissue inhibitor of metalloproteinases-2 (TIMP-2) were unaffected by either VEGF-A or marmesin treatment. Matrix metalloproteinase-9 (MMP-9) was not clearly detectable in the conditioned media. Additionally, marmesin suppressed VEGF-A-induced formation of capillary-like structures and microvessel sprouting, suggesting that its inhibition of MMP-2 contributes to the reduced migratory and invasive potential of endothelial cells. These findings highlight the pharmacological potential of marmesin in regulating VEGF-A-induced endothelial cell proliferation, migration, invasion, tube formation, and angiogenic sprouting[8].

Anti-inflammatory activity of Marmesin:

Kim JS et al 2006 has investigated that chemical Constituents of the Root of Dystaenia takeshimana isolated five coumarins (including scopoletin and (+)-marmesin) and three flavonoids. These compounds displayed dual inhibitory effects against two key inflammatory enzymes:

Cyclooxygenase-2 (COX-2)

5-Lipoxygenase (5-LOX)

Where, COX-2 is central to prostaglandin formation (e.g., PGE_2), which drives pain and inflammation.

5-LOX leads to leukotriene (e.g., LTB_4) production, also fueling inflammatory pathways.

Data on (+)-Marmesin according to the findings was shown COX-2 inhibition was 61.2% and 5-LOX inhibition was 56.7%.

By blocking both, compounds like (+)-marmesin can:

Suppress multiple inflammatory mediators simultaneously.

Possibly reduce side effects compared to selective COX-2 inhibitors (e.g., fewer gastric or cardiovascular concerns)[9].

Hepatoprotective activity:

Jain M. et al. (2012) evaluated the potential cytotoxicity of *Feronia limonia* (F. limonia) root bark extract and its isolated compounds, considering the common presence of natural toxicants in herbal preparations. The study demonstrated that both the extract and compounds were non-toxic up to a concentration of 200 mg/mL, justifying further investigation into their hepatoprotective properties. Human hepatocellular carcinoma cell line (HepG2), a widely used in-vitro model for liver studies due to its human origin and relevance to hepatic function, was employed to assess liver protection. Carbon tetrachloride (CCl_4) exposure significantly increased aspartate aminotransferase (AST) and alanine aminotransferase (ALT) leakage, along with reduced cell viability, indicating hepatocellular damage. Co-treatment with specific fractions (FRB-7) and an isolated compound (MR-1) effectively reduced enzyme leakage and improved cell viability compared to other tested fractions (FRB-1, FRB-9, FRB-10). These hepatoprotective effects were attributed to the strong antioxidant potential of FRB-7 and MR-1, as confirmed by the 2,2-diphenyl-1-picrylhydrazyl (DPPH) assay. Phytochemical analysis revealed that FRB-7 is rich in phenolic and flavonoid compounds, while MR-1 is a coumarin—both known for their free radical scavenging activities. The promising in-vitro results support further in-vivo investigation to validate their therapeutic potential[10].

Photobiological activity of marmesin:

In a seminal study by **Uwaifo and Heidelberge at al 1983** Marmesin (5-β-hydroxyisopropyl-4,5-dihydrofurocoumarin), a linear dihydrofurocoumarin isolated from various plant sources,

for its photobiological effects on Chinese hamster V79 cells. The study demonstrated that marmesin itself was not inherently cytotoxic in the absence of light, but upon exposure to UVA radiation, it exhibited marked phototoxicity. This phototoxic response was characterized by reduced cell survival and DNA damage, suggesting that marmesin undergoes photoactivation, likely forming reactive intermediates or DNA adducts that impair cellular function. Importantly, this study helped establish the mechanistic basis of furocoumarins as photosensitizers, supporting their potential utility in photochemotherapy and photodynamic therapy. The findings also emphasized the role of hydroxyl substitution and structural conformation in modulating the light-induced biological activity of coumarin derivatives[11].

Inactivation of aldose reductase by natural coumarins: molecular insights and experimental validation:

Kamel EM, Othman SI et al 2025 conducted a comprehensive study to evaluate the inhibitory effects of six coumarin derivatives on aldose reductase (AR) using both computational and experimental strategies. Through molecular docking, molecular dynamics simulations, and Molecular Mechanics/Poisson–Boltzmann Surface Area (MM/PBSA) binding free energy calculations, auraptene, marmesin, and isopimpinellin emerged as the top candidates, showing notable binding energies of −34.88, −29.40, and −20.31 kcal/mol, respectively. Pharmacokinetic profiling via ADMET analysis indicated that all three compounds possess favorable properties, including good oral absorption and bioavailability. Enzymatic inhibition assays validated auraptene as the most effective AR inhibitor with an IC_{50} of 1.43 ± 0.14 μM, demonstrating superior efficacy compared to the reference compound quercetin (IC_{50} = 2.50 ± 0.31 μM). Marmesin and isopimpinellin followed, with IC_{50} values of 3.80 ± 0.1 μM and 5.71 ± 0.8 μM, respectively. Further kinetic analysis revealed different modes of inhibition: auraptene exhibited noncompetitive inhibition (Ki = 1.84 μM), isopimpinellin showed competitive inhibition (Ki = 1.83 μM), while marmesin functioned as a mixed-type inhibitor (Ki = 2.32 μM). Collectively, these findings propose auraptene and marmesin as promising lead compounds for the development of AR inhibitors, potentially useful in the treatment of diabetic complications[12].

Antimycobacterial activity:

Suja KP, Jose L et al 2017 investigated that the potential of Bael fruit as a source of antimycobacterial agents. Using solvent extraction and chromatographic techniques, the

researchers isolated six bioactive compounds—imperatorin, β-sitosterol, plumbagin, marmesin, marmin, and stigmasterol—from the hexane fraction of the fruit extract. These compounds were tested against *Mycobacterium tuberculosis* H37Rv using a resazurin microtiter assay, and all exhibited inhibitory activity with a minimum inhibitory concentration (MIC) of approximately 50 µg/mL. Importantly, cytotoxicity assays using THP-1 derived human macrophages showed that these compounds were non-toxic at effective doses. The findings highlight the fruit's pharmacological promise and support its traditional use in treating respiratory infections, suggesting that these natural compounds could serve as lead candidates in the development of novel antitubercular drugs[13].

In vitro and in vivo anticancer effects of marmesin in U937 human leukemia cells:

Marmesin, a naturally occurring coumarin, **Dong L, Xu WW et al 2018** reported to exhibit significant anticancer activity against U937 human leukemia cells through multiple mechanisms. It demonstrated selective cytotoxicity, with lower toxicity toward normal monocytes, and inhibited leukemia cell proliferation by inducing apoptosis via the mitochondrial pathway evidenced by increased reactive oxygen species (ROS), disrupted mitochondrial membrane potential, and an elevated Bax/Bcl-2 ratio. Additionally, marmesin caused cell cycle arrest at the G_2/M phase and suppressed cancer cell migration. In vivo, tumor growth inhibition was observed in mouse xenograft models following marmesin treatment[14].

Antimicrobial activity:

Dikpınar T, Süzgeç-Selçuk S et al 2018 has evaluated the antimicrobial properties of *Ferulago trachycarpa* (Apiaceae) rhizome extracts, prepared using n-hexane, dichloromethane, and methanol through both sequential and direct extraction methods. Using the microdilution method, these extracts were tested against a panel of bacterial strains—including *Staphylococcus aureus* (ATCC 6538), *S. epidermidis*, *Escherichia coli*, *Klebsiella pneumoniae*, *Pseudomonas aeruginosa*, *Proteus mirabilis*, and *Enterococcus faecalis*—as well as fungal strains such as *Candida albicans*, *C. tropicalis*, and *C. parapsilosis*. All extracts demonstrated varying degrees of antimicrobial activity, with the n-hexane and dichloromethane fractions showing the strongest effects, prompting the isolation of active constituents from these two extracts. Four coumarin-based compounds were successfully isolated: crenulatin (6-formyl-7-methoxycoumarin), suberosin (7-methoxy-6-prenylcoumarin), marmesin senecioate [(-)-prantschimgin], and ulopterol [6-(2',3'-

dihydroxy-3'-methylbutyl)-7-methoxycoumarin]. Among these, crenulatin, suberosin, and marmesin senecioate exhibited notable antifungal activity against *C. albicans* with MIC values of 625 mg/L, and antibacterial activity against methicillin-resistant *S. aureus* (MRSA) with MIC values of 1250 mg/L. These findings suggest that F. trachycarpa, along with its coumarin derivatives, holds promising potential for development into antimicrobial agents[15].

CONCLUSION

Marmesin, a naturally occurring furanocoumarin, exhibits a remarkable spectrum of pharmacological activities supported by both experimental and computational studies. Its therapeutic potential spans across diverse biological systems, demonstrating anticancer, antidiabetic, anti-inflammatory, hepatoprotective, antiplasmodial, antimicrobial, and photobiological effects. Mechanistically, marmesin exerts its actions through multiple molecular pathways, including modulation of PI3K/Akt signaling, VEGF-A inhibition, COX-2 and 5-LOX suppression, and HSULF-2 blockade, highlighting its ability to influence critical targets in disease progression.

Despite promising in vitro and in vivo findings, further toxicological profiling, pharmacokinetic evaluation, and clinical validation are essential to translate its preclinical efficacy into therapeutic applications. The compound's structural simplicity, natural abundance, and multitarget pharmacology make it an attractive scaffold for drug design and development of novel therapeutics against cancer, metabolic, and inflammatory disorders. Overall, marmesin represents a potent bioactive molecule that bridges traditional medicine and modern pharmacological innovation, warranting deeper exploration for its integration into future drug discovery pipelines.

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